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Mechanism of lithium and magnesium oxides (LixOx and MgxOx) adsorption onto pristine graphene: Density functional theory approach

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We computationally investigated the adsorption behaviour of lithium oxides (LixOx) and magnesium oxides (MgxOx) onto pristine graphene during oxygen reduction reaction (ORR) for lithium air batteries operation using density functional theory (DFT). We proposed various pathways and studied different adsorption configurations in each system, comprising the O2, Li, and Mg as ORR reactants and the LiO2, MgO2, Li2O2 and Mg2O2 as ORR products. Mg atom weakly adsorbed onto graphene with an adsorption energy of (-0.035 eV to -0.043 eV), followed by O2 molecule (-0.101 eV to -0.134 eV) moreover Li atom adsorbed strongly with an adsorption energy of (-0.985 eV to -1.296 eV). The ORR product MgO2 adsorbed strongly with an adsorption energy of(-1.536 eV) than other reaction products LiO2, Li2O2 and Mg2O2 with their calculated adsorption energies of (+0.768 eV, -0.535 eV and -0.879 eV) respectively onto graphene. lastly the electronic properties (TDOS and PDOS) were calculated to understand their electronic behaviour.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

MSc

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